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Instructions for Use

Starter Kit for MALDI-TOF MS

For calibration and testing of matrix-assisted laser desorption and ionization time-of-flight mass spectrometers (MALDI-TOF MS)

Product description

The kit provides a range of standard peptides and proteins for the purpose of calibration and testing of MALDI-TOF mass spectrometers. This kit is designed to provide standards for most protein and peptide applications. Recrystallized matrices (tube 1-3) with high purity are supplied.

A combination of peptides (tube 4) provides good calibration across a typical molecular mass range between ~1000 and 3500 Da. Two mixtures of proteins (tube 5+6) allow instrument testing and calibrations for the molecular mass range between ~3000 and 70000 Da.

A special mixture of different polypeptide chain fragments (tube 7) was produced by the tryptic digest of bovine serum albumin. Three single peptides (tube 8-10) are provided for adjustment of the mass spectrometer and complete the kit.

All of the standards and matrices in the kit may also be purchased as individual components using the part number listed in the Ordering Information part at the end of this document. The components were investigated and tested on a Bruker Daltonics MALDI-TOF mass spectrometer.

Kit components

Tube	Substance	Amount
	Matrices	
1	α-Cyano-4-hydroxycinnamic acid (HCCA)	200 mg
2	Sinapinic acid (SA)	200 mg
3	2,5-Dihydroxybenzoic acid (2,5-DHB)	200 mg

Tube	Substance	Amount
	Peptide / protein standards	
4	Peptide calibration standard	for 250 calibration spots
5	Protein calibration standard I	for 250 calibration spots
6	Protein standard II	for 250 spots
7	Tryptic digest of bovine serum albumin	for 250 spots
	Peptides	
8	Angiotensin II	500 pmol
9	ACTH 18 – 39	500 pmol
10	Somatostatin 28	500 pmol

Storage and stability

The kit is shipped at ambient temperatures. We recommend storing all components on arrival at less than 0 °C. Sample solutions should be aliquoted and frozen. We do not recommend refreezing samples after thawing.

Risk and safety information

The kit has to be labeled according to Regulation (EC) No 1272/2008. It contains components that are classified as hazardous chemical (Signal words: DANGER and WARNING). Please read the Material Safety Data Sheet which is available for download at www.bruker.com/msds in the product description area.

Beside the kit components, we recommend further chemicals within these Instructions for Use. Please read and observe the respective Material Safety Data Sheet to be provided by your supplier. Observe the general safety regulations when handling chemicals.

Characterization and measurement results of peptide calibration standard

The next table contains molecular weights of all components in the peptide mixtures (peptide calibration standard). Fig. 1 shows results of measurement.

Peptide	$[M+H]^+$ Mono isotopic	$[M+H]^+$ Average
Angiotensin II	1046.5418	1047.19
Angiotensin I	1296.6848	1297.49
Substance P	1347.7354	1348.64
Bombesin	1619.8223	1620.86
ACTH clip 1-17	2093.0862	2094.43
ACTH clip 18-39	2465.1983	2466.68
Somatostatin 28	3147.4710	3149.57

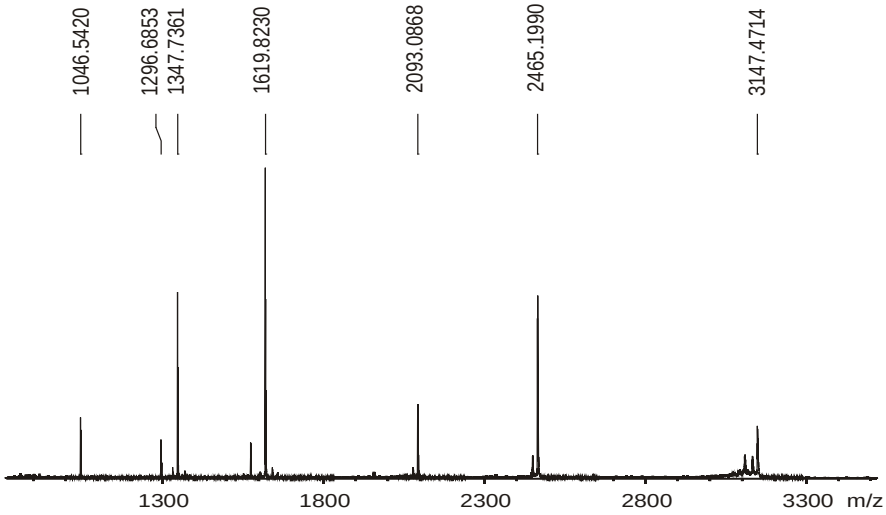

Fig. 1: MALDI mass spectrum of peptide calibration standard. Target preparation with HCCA matrix.

Characterization and measurement results of protein calibration standards

The kit contains two different protein mixtures (I and II) as test and calibration standards with following compositions.

Protein standard I	Average m/z	Protein standard II	Average m/z
Insulin $[M+H]^+$	5734.51	Trypsinogen $[M+H]^+$	23982
Ubiquitin $[M+H]^+$	8565.76	Protein A $[M+H]^+$	44613
Cytochrome C $[M+H]^+$	12360.97	Albumin-Bovine $[M+H]^+$	66431*
Myoglobin $[M+H]^+$	16952.30	Protein A $[M+2H]^{2+}$	22306
Cytochrome C $[M+2H]^{2+}$	6180.99	Albumin-Bovine $[M+2H]^{2+}$	33216*
Myoglobin $[M+2H]^{2+}$	8476.65		

* Bovine serum albumin is not recommended for calibration purposes due to a mass shift to higher m/z values caused by unspecific adduct formation (s. Fig. 4). If an instrument calibration in a higher m/z range is required, we advise an extrapolation of a linear calibration based on the signals at m/z 22306, 23982 and 44613.

The next two figures 2 and 3 show different spectra of protein calibration standard I due to different preparations of MALDI-TOF targets.

Fig. 4 shows the spectrum of protein calibration standard II. The target was preloaded with SA.

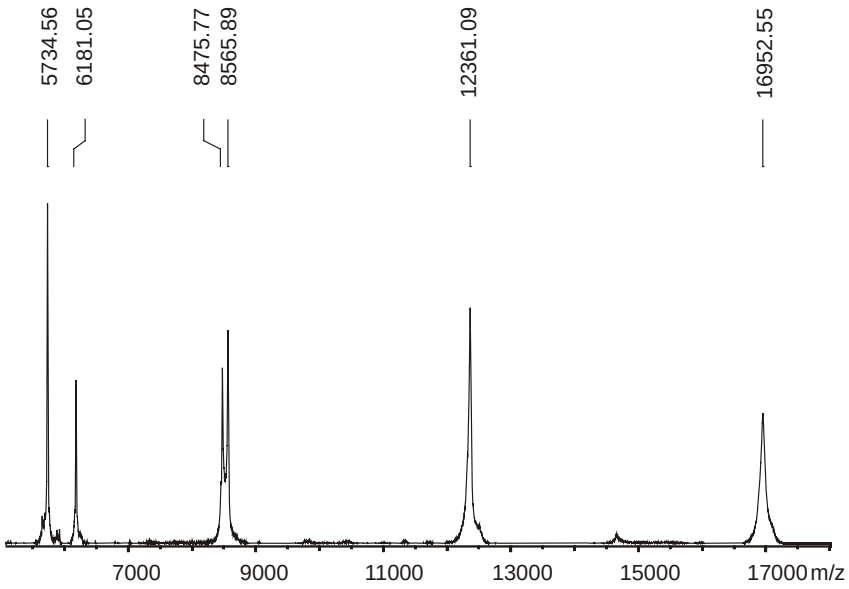

Fig. 2: MALDI mass spectrum of protein calibration standard I. Target preparation with HCCA matrix.

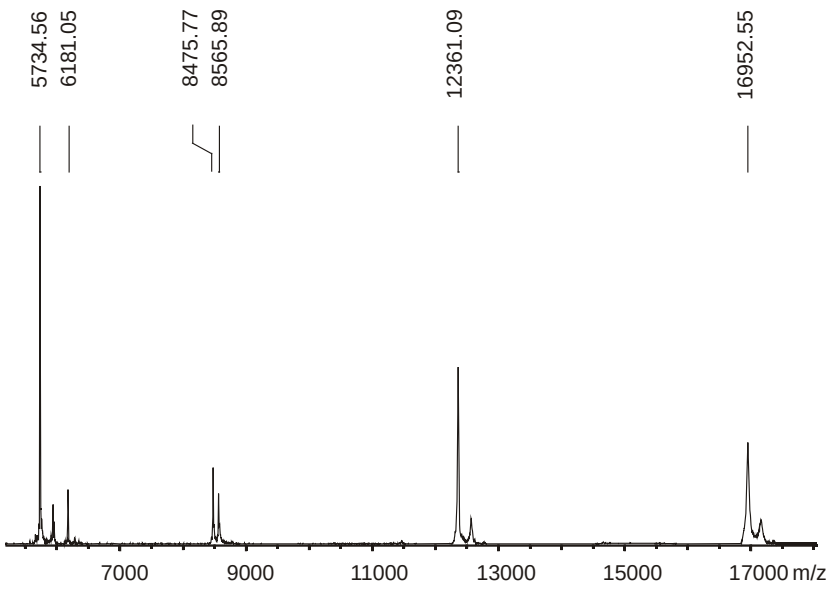

Fig. 3: MALDI mass spectrum of protein calibration standard I. Target preparation with SA matrix.

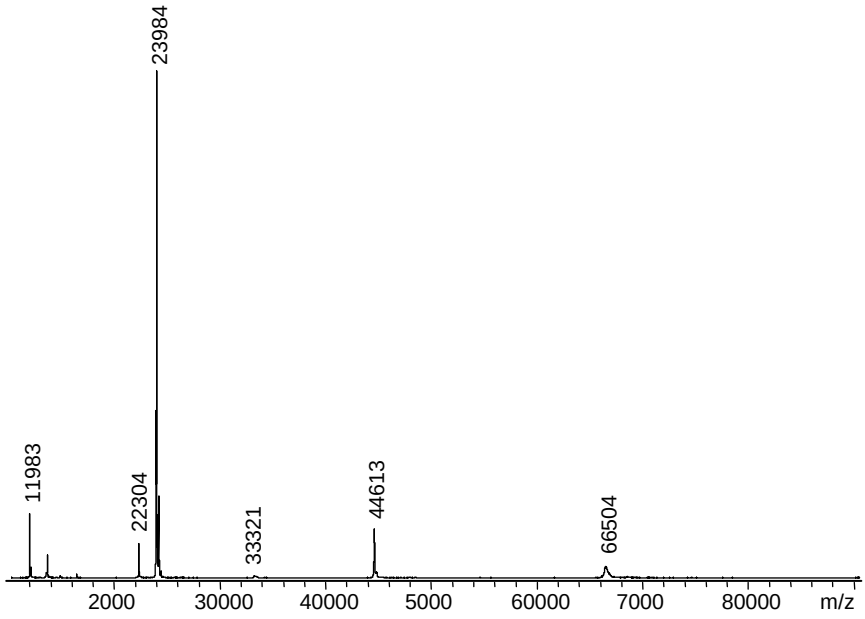

Fig. 4: MALDI mass spectrum of protein calibration standard II. Target preparation with SA matrix, linear calibration with protein A (1- and 2-fold charged) and trypsinogen (1-fold charged).

Characterization and measurement results of tryptic digest of bovine serum albumin

Different proteolytic polypeptides characterize the tryptic digest of bovine serum albumin (BSA). In the next table the different peptides and molecular masses are listed. Figure 5 depicts a typical MALDI-TOF spectrum of the BSA digest.

Fragments	$[M+H]^+$ Mono isotopic	$[M+H]^+$ Average
Intact protein		66431.00
[161 – 167]	927.493	928.06
[66 – 75]	1163.631	1164.33
[361 – 371]	1283.711	1284.49
[402 – 412]	1305.716	1306.49
[569 – 580]	1399.693	1400.62
[360 – 371]	1439.812	1440.67
[421 – 433]	1479.795	1480.69
[347 – 359]	1567.743	1568.71
[437 – 451]	1639.938	1640.90
[347 – 360]	1723.844	1724.89
[508 – 523]	1880.921	1882.13
[529 – 544]	1907.921	1909.15
[168 – 183]	2045.028	2046.31

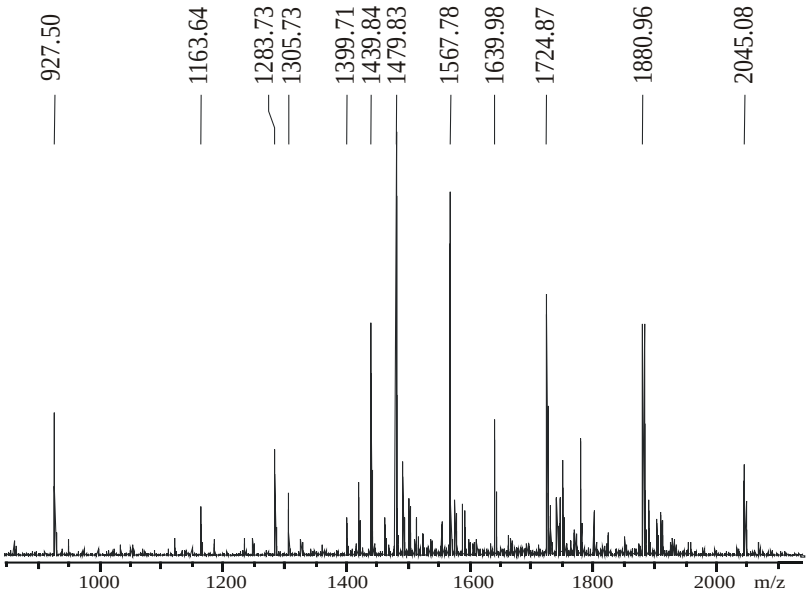

Fig. 5: MALDI mass spectrum of tryptic digest of bovine serum albumin. Anchor-Chip™ target preparation with HCCA matrix.

Sample preparation procedure (recommendation)

Pre-Remarks

Poor sample preparation will degrade sensitivity, yield low resolution and poor reproducibility. The generation of ions through MALDI depends on the production of a suitable composite material, consisting of the matrix substance and the analyte. For best results use only chemicals of highest available purity.

Chemicals and materials required

Acetonitrile (ACN)
0.1% Trifluoroacetic acid (0.1% TFA) in water

: Acetonitrile is classified as hazardous chemical (DANGER: H: 225, 319, 302, 312, 332; P: 210, 280, 305+351+338).

Necessary equipment and tools: centrifuge, shaker, ultra sonic device, pipettes, pipette tips

1. Preparation of sample solution

Dissolve samples (whole contents of tubes 4-10) in each case in 125 µL 0.1% TFA solvent and shake for several seconds.

2. Preparation of matrix solution

Produce a mix of ACN and 0.1% TFA in a volume ratio 1:2. Solve HCCA, SA or 2,5-DHB in this solvent up to saturation at room temperature. Assist the solution process by help of ultrasonic device. Spin down excess matrix in a centrifuge (5 min at 14000 rpm) and use only the homogeneous transparent phase. Use matrix solutions according our recommendations in the following table.

Tube	Sample	Matrix
4	Peptide calibration standard	HCCA, 2,5-DHB
5	Protein calibration standard I	HCCA, SA, 2,5-DHB
6	Protein calibration standard II	SA, 2,5-DHB
7	Tryptic digest of bovine serum albumin	HCCA, 2,5-DHB
8	Angiotensin II	HCCA, 2,5-DHB
9	ACTH, clip 18-39	HCCA, 2,5-DHB
10	Somatostatin 28	HCCA, 2,5-DHB

3. Preparation onto MALDI-TOF-Target

According to the dried droplet method, mix equal volumes of sample and matrix solution (HCCA, SA or 2,5-DHB). Apply 1 µL onto a standard steel target and dry at room temperature.

For AnchorChip™ target preparation, refer to the AnchorChip Instructions for Use (# 8215344).

Ordering Information

Product	Part No.	Size
Starter Kit	8208241	
α-Cyano-4-hydroxycinnamic acid (HCCA)	8201344	5 x 200mg
Sinapinic acid (SA)	8201345	5 x 200mg
2,5-Dihydroxybenzoic acid (2,5-DHB)	8201346	5 x 200mg
Peptide calibration standard	8206195	for 5 x 250 calibration spots
Peptide calibration standard II	8222570	for 5 x 250 calibration spots
Protein calibration standard I	8206355	for 5 x 250 calibration spots
Protein standard II	8207234	for 5 x 250 spots
Tryptic digest of bovine serum albumin	8217498	for 5 x 250 spots

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